# Early SCIENCE Program

at the Argonne Leadership Computing Facility

Allocations through the Early Science Program (ESP) provide researchers with preproduction hours (between system installation and full production) on the ALCF's next-generation, 10 petaflops IBM Blue Gene system, Mira. This early science period provides projects with a significant head start for adapting to the new machine and access to substantial computational time. During this shakedown period, users assist in identifying the root causes of any system instabilities, and work with ALCF staff to help develop solutions. More than two billion core hours are allocated through ESP. For more information, visit: http://esp.alcf.anl.gov.



Climate-Weather Modeling Studies Using a Prototype Global Cloud-System Resolving Model

PI: Venkatramani Balaji Geophysical Fluid Dynamics Laboratory Award: 150 Million Hours



Materials Design and Discovery: Catalysis and Energy Storage

PI: Larry Curtiss Argonne National Laboratory Award: 50 Million Hours



Direct Numerical Simulation of Autoignition in a Jet in a Cross-Flow

PI: Christos Frouzakis Swiss Federal Institute of Technology Award: 150 Million Hours



High-Accuracy Predictions of the Bulk Properties of Water

PI: Mark Gordon lowa State University Award: 150 Million Hours



Cosmic Structure Probes of the Dark Universe

PI: Salman Habib Los Alamos National Laboratory Award: 150 Million Hours



Accurate Numerical Simulations of Chemical Phenomena Involved in Energy Production and Storage with MADNESS and MPQC

PI: Robert Harrison Oak Ridge National Laboratory Award: 150 Million Hours



Petascale, Adaptive CFD

PI: Kenneth Jansen University of Colorado-Boulder Award: 1.50 Million Hours



Using Multi-scale Dynamic Rupture Models to Improve Ground Motion Estimates

PI: Thomas Jordan University of Southern California Award: 150 Million Hours



## at the Argonne Leadership Computing Facility



# High-Speed Combustion and Detonation (HSCD)

PI: Alexei Khokhlov The University of Chicago Award: 150 Million Hours



### Petascale Simulations of Turbulent Nuclear Combustion

PI: Don Lamb The University of Chicago Award: 150 Million Hours



### Lattice Quantum Chromodynamics

PI: Paul Mackenzie Fermilab

Award: 150 Million Hours



# Petascale Direct Numerical Simulations of Turbulent Channel Flow

PI: Robert Moser University of Texas

Award: 60 Million Hours



# Ab-initio Reaction Calculations for Carbon-12

PI: Steven C. Pieper Argonne National Laboratory Award: 110 Million Hours



### NAMD - The Engine for Large-Scale Classical MD Simulations of Biomolecular Systems Based on a Polarizable Force Field

PI: Benoit Roux The University of Chicago Award: 80 Million Hours



### Global Simulation of Plasma Microturbulence at the Petascale and Beyond

PI: William Tang Princeton Plasma Physics Laboratory

Award: 50 Million Hours



# Multiscale Molecular Simulations at the Petascale

PI: Gregory Voth The University of Chicago Award: 150 Million Hours

